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ABSTRACT

Some L-stable fourth order explicit one step numerical integration formulas which require no matrix inversion are proposed to cope effectively with systems of ordinary differential equations with large Lipschitz constants (including those having highly oscillatory solutions). The implicit integration procedure proposed in Fatunla [10] is further developed to handle a larger class of stiff systems as well as those with highly oscillatory solutions. The same pair of nonlinear equations as in [10] is solved for the stiffness/oscillatory parameters. However, the nonlinear systems are transformed into linear forms and an efficient computational procedure is developed to obtain these parameters. The new schemes compare favorably with the backward differentiation formula (DIFSUB) of Gear [12, 13] and the blended linear multistep methods of Skeel and Kong [22], and the symmetric multistep methods of Lambert and Watson [16].

1. INTRODUCTION

The development of numerical integration formulas for stiff as well as highly oscillatory systems of differential equations has attracted considerable attention in the past decade. The reason for this cannot be farfetched, realizing that the mathematical models of physical situations in kinetic chemical reactions, process control and electrical circuit theory often generate systems of ordinary differential equations whose Jacobians have at least one eigenvalue with a very negative real part or very large imaginary part. Both situations are respectively described as stiff and highly oscillatory.

Consider the following model problems

(1.1) $$y' = \lambda(y-c(x)) + c'(x),$$

$$y(a) = y_0,$$

where $y(x) \in R^1$, λ a complex constant with re $\lambda << 0$ and $c(x)$ has the property $|c'(x)| \simeq 0$ in the finite interval $a \leq x \leq b$;

(1.2) $$z' = \begin{pmatrix} -\varepsilon & \omega \\ -\omega & -\varepsilon \end{pmatrix} z, \qquad z(a) = z_0,$$

with $z(x) \in R^2$ and $\omega >> 0$, ε a positive constant such that $\varepsilon \simeq 0$.

Problem (1.1) has theoretical solution

(1.3) $$y(x) = c(x) + y_0 e^{\lambda x}$$

whose component $c(x)$ is slowly varying in the specified interval while the second component decays rapidly in the transient phase.

The analytic solution to problem (1.2) is given by

(1.4) $$z(x) = e^{-\varepsilon x} \begin{pmatrix} \alpha \cos \omega x + \beta \sin \omega x \\ +\beta \cos \omega x - \alpha \sin \omega x \end{pmatrix}$$

where α and β are the arbitrary constants of integration.

The transitory phase for problem (1.1) is of the order of $-1/\lambda$ while that of problem (1.2) is the entire interval of integration with $\omega/2\pi$ complete oscillations per unit interval.

Almost invariably, most conventional numerical integration solvers cannot effectively cope with problems (1.1) and (1.2) as they lack adequate stability characteristics. Any attempt to impose the stability properties will in effect constrain the integration mesh-size to be intolerably small. This may ultimately have adverse effects on the accuracy due to propagation of roundoff errors. Besides, the computing time and cost may be too excessive.

Existing algorithms developed for problems of the type (1.1) can be classified into the following categories:

(i) generalized Runge-Kutta schemes

(ii) implicit Runge-Kutta schemes

(iii) trapezoidal rule with extrapolation

(iv) multiderivative multistep formulas

(v) backward differentiation multistep formulas.

As of now the most widely used numerical integration code for stiff systems is the class (v) schemes particularly Gear's DIFSUB [12, 13]. The method is efficient and reliable provided the eigenvalues of the Jacobian are not close to the imaginary axis where the higher order schemes exhibit poor stability properties (as evidenced from example 2). Dahlquist [5] established that neither an explicit linear multistep scheme of any order nor an implicit multistep method of order greater than two can be A-stable. He proved that the trapezoidal rule (which of course is not L-stable as $y_t/y_{t-1} \to 1$ as $\lambda h \to -\infty$) has the smallest error of $(\pm)\frac{1}{12} h^3 y^{(3)}_{(x)}$. Other schemes which behave better than DIFSUB when the eigenvalues are close

to the imaginary axis includes the second derivative multistep method Enright [6].

As regards problems of the type (1.2), earlier efforts include Gautschi's [11] nonlinear multistep schemes which produce exact solution to algebraic (or trigonometric) polynomials up to certain degrees. The main drawback of this scheme is that it requires an a priori knowledge of the period of the systems under consideration. Other numerical integration solvers to oscillatory systems include Amdursky and Ziv [1, 2, 3], Snider and Flemming [23], Miranker, et al. [18], Miranker and Wahba [19], Miranker and Veldhuizen [21], and Fatunla [8, 9]. Unfortunately, none of these existing routines has been properly (adequately) put to test for various kinds of oscillatory problems.

In this paper, we propose some two-point numerical integration formulas which effectively cope with systems of ODEs whose characteristics are identical to problems (1.1) and (1.2).

We shall consider initial value problems

(1.5) $$y' = f(x,y),\ y(0) = y_0$$

with $y(x) \in R^m$ in the finite interval $S = [0,x_f] \subset R^1$ where $x_f = Nh$ for some positive integer $N > 0$. It is assumed that $y(x)$ is sufficiently differentiable. We adopt the vector notation: $y = ({}^1y, {}^2y, \ldots, {}^my)^T$, $f = ({}^1f, {}^2f, \ldots, {}^mf)$. The numerical estimates y_t to the theoretical solution $y(x_t)$ at the points $x_t = th$, $t = 0(1)N$ are to be generated.

On every subinterval $[x_t, x_t+h]$, the theoretical solution $y(x)$ is approximated by either the interpolating function

(1.6) $$\tilde{F}(x) = (I-e^{\Omega_1 x})A - (I-e^{-\Omega_2 x})B + C,$$

A, B, and C being m-tuples with real entries, I is the identity matrix whilst Ω_1 and Ω_2 are diagonal (stiffness/oscillatory) matrices or

(1.7) $$\tilde{\tilde{F}}(x) = (I-e^{\Omega_1 x})R + (I-e^{\Omega_1^* x})R^* + S$$

where R, S are m-tuples with complex entries and (*) denotes complex conjugate.

The choice of interpolation formula is determined by equation (3.12).

The following definitions are worthwhile:

Definition 1. A one-step numerical integration scheme is considered L-stable if apart from being A-stable, when it is applied to the scalar initial value problem

(1.8) $$y' = \lambda y, \ y(0) = \eta$$

(λ being a complex constant with negative real part), the resultant numerical solution is given by

(1.9) $$y_{t+1} = \mu(\lambda h) y_t$$

with the characteristic equation $\mu(\lambda h)$ having the property:

(1.10) $$\lim_{re(\lambda h) \to \infty} |\mu(\lambda h)| = 0.$$

Definition 2. A numerical integration scheme is said to be exponentially fitted at a complex value $\lambda = \lambda_0$ if when it is applied to the initial value problem (1.8) with exact initial condition, the characteristic equation $\mu(\lambda h)$ satisfies the relation

(1.11) $$\mu(\lambda_0 h) = e^{\lambda_0 h}.$$

Liniger and Willoughby [18] and Jackson and Kenue [14] have respectively discussed A-stable one- and two-step numerical integration methods which are exponentially fitted at infinity. Both schemes ensure exponential fitting by a suitable choice of a free parameter. This approach was further extended to construct a stiffly stable k-step method of order k+2 in Enright [6].

We shall construct from both equations (1.6) and (1.7) explicit one-step numerical integration formulas of fixed order four which possess adequate stability and convergent characteristics to cope with both stiff and highly oscillatory systems of ordinary differential equations. For linear systems the interpolating functions are global in the sense that the stiffness/oscillatory matrices have constant entries which are determined by solving a set of linear equations at the first step of the integration procedure. The implicit scheme proposed in Fatunla [10] is further developed using the interpolating function (1.7). The need to solve nonlinear equations for the stiffness/oscillatory parameters is eliminated.

2. DEVELOPMENT OF THE INTEGRATION FORMULAS

Let y_{t+j} denote the numerical estimate of the theoretical solution $y(x_{t+j})$ and $x = x_{t+j}$ and adopt the notation $f_{t+j} = f(x_{t+j}, y_{t+j})$ and set

(2.1) $$y_{t+j} = \tilde{F}(x_{t+j}), \qquad j = 0, 1$$

and

(2.2) $$f_t^{(k)} = \tilde{F}^{(k)}(x_t), \qquad k = 0, 1.$$

The imposition of these constraints on the interpolating function (1.6) gives the integration formula

(2.3) $$y_{t+1} = y_t + rf_t + sf_t^{(1)},$$

where

(2.4) $$r = (\Omega_2\gamma - \Omega_1\sigma),$$

and

(2.5) $$s = \gamma + \sigma;$$

γ and σ are diagonal matrices with entries

(2.6) $${}^i\gamma = \frac{e^{{}^i\Omega_1 h} - 1}{{}^i\Omega_1({}^i\Omega_1 + {}^i\Omega_2)}, \qquad i = 1(1)m,$$

and

(2.7) $${}^i\sigma = \frac{(e^{-{}^i\Omega_2 h} - 1}{{}^i\Omega_2({}^i\Omega_1 + {}^i\Omega_2)}, \quad i = 1(1)m.$$

In the event that a component of the stiffness/oscillatory matrix (${}^j\Omega_1$ say) does vanish, by L'hopital rule, the corresponding component of γ in (2.4) is

(2.8) $${}^j\gamma = \frac{h}{{}^j\Omega_2},$$

and the resultant integration formula is given by

(2.9) $$^{j}y_{t+1} = {}^{j}y_{t} + h\,{}^{j}f_{t} + \left(\frac{h}{^{j}\Omega_2} + {}^{j}\sigma\right){}^{j}f_{t}^{(1)} .$$

We now consider the case of the complex interpolating function (1.7). Let the parameters be expressed as

(2.10) $$\Omega_1 = \lambda + iu$$

and

$$\Omega_1^* = \lambda - iu$$

By imposing constraints (2.1) and (2.2) on (1.7), we obtained the integration formula (2.3) with r and s given by

(2.11) $$r(\lambda,u) = \frac{e^{\lambda h}\{(\lambda^2-u^2)\sin(hu)-2\lambda u\cos(hu)\} + 2\lambda u}{u(\lambda^2+u^2)} ,$$

(2.12) $$s(\lambda,u) = \frac{e^{\lambda h}\{\lambda\sin(hu)-u\cos(hu)\} + u}{u(\lambda^2+u^2)}$$

Near the origin , equations (2.11) and (2.12) reduce to

(2.13) $$r(\lambda,u) = h$$

and

(2.14) $$s(\lambda,u) = \frac{h^2}{2} ,$$

and thus the integration formula (2.3) reduces to the second order Taylor series.

3. EVALUATION OF STIFFNESS PARAMETERS

By using the Taylors expansion of $y_{t+1} \equiv y(x_t+h)$ about $x = x_t$ and the Maclaurin's series of $e^{\Omega_1 h}$, $e^{-\Omega_2 h}$ in the integration formula (2.3) it is observed that the coefficients of h^0, h^1, and h^2 vanish identically. With the view to obtain numerical estimates for the stiffness/oscillatory parameters, we simply allow the coefficients of h^3 and h^4 to vanish thus yielding the following pair of nonlinear equations

(3.1) $$(\Omega_2-\Omega_1)f_t^{(1)} - \Omega_1\Omega_2 f_t = -f_t^{(2)},$$

and

(3.2) $$-(\Omega_1^2-\Omega_1\Omega_2+\Omega_2^2)f_t^{(2)} + \Omega_1\Omega_2(\Omega_2-\Omega_1)f_t^{(1)} = -f_t^{(3)} .$$

By adopting (3.1) as a definition of $\Omega_1\Omega_2 f_t$, equation (3.2) becomes

(3.3) $$(\Omega_2-\Omega_1)f_t^{(2)} - \Omega_1\Omega_2 f_t^{(1)} = -f_t^{(3)} .$$

If the set of equations (3.1) and (3.3) were to be meaningful, it is desirable that

(3.4) $$\det\begin{pmatrix} {}^i f_t^{(2)} & {}^i f_t^{(1)} \\ {}^i f_t^{(1)} & {}^i f_t \end{pmatrix} \neq 0, \qquad i = 1(1)m.$$

Let

(3.5) $${}^iD = {}^i\Omega_2 - {}^i\Omega_1, \qquad i = 1(1)m;$$

and

(3.6) $${}^iE = {}^i\Omega_1 {}^i\Omega_2 , \qquad i = 1(1)m$$

Equations (3.1) and (3.3) can now be expressed as m pairs of linear equations

$$(3.7)\qquad \begin{cases} {}^iD\,{}^if_t^{(2)} - {}^iE\,{}^if_t^{(1)} = -{}^if_t^{(3)}, \\ {}^iD\,{}^if_t^{(1)} - {}^iE\,{}^if_t \quad = -{}^if_t^{(2)}, \end{cases} \qquad \text{for } i = 1(1)m.$$

These m pairs of equations can be readily solved for ${}^iD$ and ${}^iE$ by the Cramer's rule to give

$$(3.8)\qquad {}^iD = \frac{{}^if_t\,{}^if_t^{(3)} - {}^if_t^{(1)}\,{}^if_t^{(2)}}{{}^if_t^{(1)}\,{}^if_t^{(1)} - {}^if_t\,{}^if_t^{(2)}}, \qquad i = 1(1)m$$

and

$$(3.9)\qquad {}^iE = \frac{{}^if_t^{(1)}\,{}^if_t^{(3)} - {}^if_t^{(2)}\,{}^if_t^{(2)}}{{}^if_t^{(1)}\,{}^if_t^{(1)} - {}^if_t\,{}^if_t^{(2)}}, \qquad i = 1(1)m.$$

The numerical values obtained for ${}^iD$ and ${}^iE$ can be substituted in equations (3.5) and (3.6) to generate the oscillatory/stiffness parameters as

$$(3.10)\qquad {}^i\Omega_i = \frac{1}{2}[-{}^iD + \sqrt{({}^iD^2+4\,{}^iE)}],$$

and

$$(3.11)\qquad {}^i\Omega_2 = {}^i\Omega_1 + {}^iD.$$

The complex interpolation formula (1.7) is adopted if in (3.10), the following relationship holds:

$$(3.12)\qquad {}^iD^2 < 4\,{}^iE$$

4. STABILITY CONSIDERATIONS

We now apply the integration formula (2.9) to the scalar test equation

(4.1) $$y' = \lambda y + g$$

where λ is a complex constant with negative real part and g is a real constant.

The numerical solution is given as

(4.2) $$y_{t+1} = p(\lambda,\Omega_2,h)y_t + gh$$

where the characteristic equation $p(\lambda,\Omega_2,h)$ is given by

(4.3) $$p(\lambda,\Omega_2,h) = 1 + \lambda h + \lambda^2(\Omega_2 h + e^{-\Omega_2 h} - 1)/\Omega_2^2$$

Equation (3.11) gives the following relationship:

(4.4) $$\Omega_2 = {}^{i}D = D$$

If we use equation (4.1) in (3.8), we readily obtain

(4.5) $$D = -\lambda = \Omega_2$$

This in equation (4.3) gives

(4.6) $$P(\lambda,-\lambda,h) = e^{\lambda h} .$$

We further consider the application of the integration formula (2.3) to test problem (4.1) for the case when the stiffness/oscillatory parameter is imaginary. Thus, $r(\lambda,u)$ and $s(\lambda,u)$ used in the two integration formulas (2.3) to the test problem (4.1) as specified by

(4.7) $$r(\lambda,u) = \frac{\sin(hu)}{u} ,$$

and

(4.8) $$s(\lambda,u) = \frac{1-\cos(hu)}{u^2} .$$

Let

$$\lambda = iz, \qquad i^2 = -1. \tag{4.9}$$

The resultant integration formula is given by

$$y_{t+1} = q(\lambda,u,h)y_t + gh, \tag{4.10}$$

where the characteristic equation can be obtained as

$$q(\lambda,u,h) = 1 + \frac{(1-\cos(hu))\lambda^2}{u^2} + \frac{\sin(hu)\lambda}{u} \quad . \tag{4.11}$$

The application of equation (4.1) and (4.9) in (3.8) yields

$$\begin{aligned} D &= -iz = -\lambda. \\ &= \Omega_1^*. \end{aligned} \tag{4.12}$$

This in (4.11) gives

$$\begin{aligned} q(u,u,h) &= 1 - (1-\cos(hu))+i\sin(hu) \\ &= e^{ihu} \\ &= e^{\lambda h} \quad . \end{aligned} \tag{4.13}$$

Equations (4.6) and (4.13) together with definitions 1 and 2 thus establish the L-stability and exponential fitting of the proposed integration formulas.

5. LOCAL TRUNCATION ERROR

We now associate with the integration formula (2.3) the operator $V[y(x),h]$ specified as

$$V(y(x),h) = y(x+h) - y(x) + (\Omega_2\gamma-\Omega_1\sigma)f(x,y) - (\gamma+\sigma)f^{(1)}(x,y) \tag{5.1}$$

for an arbitrary function $y(x) \in C^5(S)$. The local truncation error T_{t+1} at $x = x_{t+1}$ is hence given as $V[y(x_t),h]$ where $y(x_t)$ denotes the solution to the initial value problem (1.5). By using the Taylors expansion of $V[y(x),h]$ about $x = x_t$ with the localizing assumption that there is no previous error (i.e., $y_t = y(x_t)$), the truncation error for the integration formula (2.3) with constraints (3.1) and (3.3) can be derived at

$$T_{t+1} = \frac{h^5}{5!}\{(\Omega_1+\Omega_2)^{-1}[(\Omega_1+\Omega_2)f_t^{(4)} - \Omega_1^4(f_t^{(1)}+\Omega_2 f_t) + \Omega_2^4(f_t^{(1)}-\Omega_1 f_t)]\} + O(h^6). \tag{5.2}$$

The corresponding truncation formula for the integration formula (2.9) is given by

$$T_{t+1} = \frac{h^5}{5!}(f_t^{(4)}-\Omega_2^3 f_t^{(1)}) + O(h^6), \tag{5.3}$$

while the truncation error when $r(\lambda,u)$ and $s(\lambda,u)$ are specified by equations (2.11) and (2.12) is

$$T_{t+1} = \frac{h^5}{5!}[f_t^{(4)} + (\lambda^2+u^2)(3\lambda^2-u^2)f_t + 4\lambda(u^2-\lambda^2)f_t^{(1)}] + O(h^6). \tag{5.4}$$

From equations (5.3) and (5.4) we deduce that all the proposed explicit integration formulas are of fixed order four.

6. EXTENSION OF NONLINEAR SCHEME

We recall the implicit numerical integration formula proposed in Fatunla [10]:

$$(6.1) \qquad y_{t+1}^{[s+1]} = y_{t+1}^{[s]} - [I - J_{t+1}^{[s]}]^{-1} [y_{t+1}^{[s]} - f_{t+1}^{[s]} - G_t], \qquad s = 0, 1, 2\ldots$$

where $J_{t+1}^{[s]}$ denotes the Jacobian specified as

$$(6.2) \qquad J_{t+1}^{[s]} = \frac{\delta f}{\delta j}(x_{t+1}, y_{t+1}^{[s]}), \quad f_{t+1}^{[s]} = f(x_{t+1}, y_{t+1}^{[s]}),$$

and

$$(6.3) \qquad G_t = y_t - (\gamma + \sigma) f_t.$$

The components of θ, γ, σ are obtained as

$$(6.4) \qquad {}^i\theta = \frac{{}^i\Omega_2(1-e^{{}^i\Omega_1 h}) + {}^i\Omega_1(1-e^{-{}^i\Omega_2 h})}{{}^i\Omega_1\,{}^i\Omega_2(e^{-{}^i\Omega_2 h} - e^{{}^i\Omega_1 h})}, \qquad i = 1(1)m,$$

$$(6.5) \qquad {}^i\gamma = \frac{e^{-{}^i\Omega_2 h}(1-e^{{}^i\Omega_1 h})}{{}^i\Omega_1(e^{-{}^i\Omega_2 h} - e^{{}^i\Omega_1 h})}, \qquad i = 1(1)m,$$

and

$$(6.6) \qquad {}^i\sigma = \frac{e^{{}^i\Omega_1 h}(1-e^{-{}^i\Omega_2 h})}{{}^i\Omega_2(e^{-{}^i\Omega_2 h} - e^{{}^i\Omega_1 h})}, \qquad i = 1(1)m.$$

The corresponding truncation error for the integration formula (6.1) was obtained as

$$(6.7) \qquad T_{t+1} = \frac{h^6}{720}\{9f_t^{(4)} + t(\Omega_2-\Omega_1)f_t^{(3)} + 5(\Omega_1^2-\Omega_1\Omega_2+\Omega_2^2)f_t^{(2)}$$

$$- 9(\Omega_2-\Omega_1)(\Omega_1^2+\Omega_2^2)f_t^{(1)}$$

$$+ [5\Omega_1^2\Omega_2^2 - 9\Omega_1\Omega_2(\Omega_1^2-\Omega_1\Omega_2+\Omega_2^2)]f_t] + 0(h^7).$$

In the case when the oscillatory/stiffness parameters have complex values, the components of θ and $(\gamma+\delta)$ in equation (6.1) are replaced by

$$(6.8) \qquad {}^{i}\theta = \frac{e^{\lambda h}[u\cos(hu) - \lambda\sin(hu)] + u}{e^{\lambda h}(\lambda^2+u^2)\sin(hu)}, \qquad i = 1(1)m$$

$$(6.9) \qquad {}^{i}(\gamma+\delta) = \frac{ue^{\lambda h} - [\lambda\sin(hu) + u\cos(hu)]}{(\lambda^2+u^2)\sin(hu)}$$

with the truncation error (6.7) replaced by

$$(6.10) \qquad T_{t+1} = \frac{h^6}{720}\{9f_t^{(4)} - 10\lambda f_t^{(3)} + 5(3\lambda^2-u^2)f_t^{(2)} + 36(\lambda^2-u^2)f_t^{(1)} + 4(\lambda^2+u^2)(8\lambda^2-u^2)f_t\} + O(h^7)\,.$$

7. NUMERICAL EXAMPLES

Example 1

We first consider the linear system:

$$(7.1) \qquad y' = \begin{bmatrix} -.1 & -49.9 & 0 \\ 0 & -50 & 0 \\ 0 & 70 & -120 \end{bmatrix} y, \qquad y(0) = \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix}$$

in the interval $0 \leq x \leq 15$. The eigenvalues of the Jacobian of (7.1) are $\lambda_1 = -0.1$, $\lambda_2 = -50$, $\lambda_3 = -120$. The theoretical solution is given as

$$^1y(x) = e^{-0.1x} + e^{-50x}$$

$$^2y(x) = e^{-50x}$$

$$^3y(x) = e^{-50x} + e^{-120x}.$$

The new explicit scheme performs better than the DIFSUB [13] and the blended DIFSUB [22]. Details of the numerical results are given in Table 7.1.

TABLE 7.1. Numerical Results for Example 1.

Method	Max Order	Steps	Function Calls	Back Solves	LU Decomp	Accurate Digits
DIFSUB	6	353	1024	969	18	9.3
BLENDED DIFSUB	11	234	595	1056	22	10.4
EXPLICIT SCHEME	4	75	75	-	-	12.5

Example 2

We further consider the linear problem:

$$(7.2)\qquad y' = \begin{bmatrix} -10 & 100 & 0 & 0 & 0 & 0 \\ -100 & -10 & 0 & 0 & 0 & 0 \\ 0 & 0 & -4 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -.5 & 0 \\ 0 & 0 & 0 & 0 & & -.1 \end{bmatrix} y, \qquad y_i(0) = 1, \quad i = 1(1)6$$

in the range $0 \leq t \leq 20$. The eigenvalues of the Jacobian are $\lambda_{1,2} = -10 \pm 100i$, $\lambda_3 = -4$, $\lambda_4 = -1$, $\lambda_5 = -.5$, and $\lambda_6 = -.1$. This problem is particularly troublesome for both DIFSUB and the blended DIBSUB as can be seen from Table 7.2.

TABLE 7.2. Numerical Results for Example 2.

ϵ	Max Order	Steps	Func Eval	Back Solves	LU Decomp	Accurate Digits
			DIFSUB			
10^{-2}	(4)	(1001)	(3002)	(2959)	(7)	(1.1)
"too much work"; integration abandoned at x = 8.3						
			blended DIFSUB			
10^{-10}	(12)	(1001)	(2917)	(5580)	(21)	(10.3)
"too much work"; integration abandoned at t = 5.1						
			Explicit Scheme			
unspec-ified	4	200	200	-	-	14.2

Example 3

We now consider the initial value problem of Liniger and Willoughby [18]:

$$(7.3a)\qquad y' = \begin{pmatrix} -2000 & 1000 \\ 1 & -1 \end{pmatrix} y + \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad y(0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

in the interval $0 \leq x \leq 5$.

This problem is contained in the test batch recommended by Bjurel, et al. [4], and was also considered in Lambert [15]. In addition, it is solved with the blended DIFSUB [22].

The eigenvalue of the Jacobian to (7.3a) are $\lambda_1 = -2000.5$ and $\lambda_2 = -0.5$ thus yielding a stiffness ratio 4001. The stiffness matrices which have constant entries were obtained as

$$(7.3b)\qquad \Omega_1 = \begin{pmatrix} -0.499875 & 0 \\ 0 & -0.499875 \end{pmatrix}, \qquad \Omega_2 = \begin{pmatrix} 2000.5 & 0 \\ 0 & 2000.5 \end{pmatrix}.$$

Table (7.3) gives the numerical results for the explicit scheme, Lambert's scheme and the blended DIFSUB. The global relative error for the blended DIFSUB is 0.743400 D-5 while the global relative error for the explicit scheme is 0.5746777037 E-05. The computational cost and function evaluation on IBM 360/75 for the blended DIFSUB are respectively \$1.84 and 107 while that of the explicit scheme is \$0.77 and 10, respectively.

The global errors were computed as

$$(7.3c)\qquad \bar{e} = \max_{0 \leq t \leq N} \left[\sum_{i=1}^{m} \left(\frac{{}^{i}y_t - {}^{i}y(x_t)}{{}^{i}\omega} \right)^2 \right]^{1/2},$$

$$(7.3d)\qquad {}^{i}\omega = \max_{1 \leq i \leq m} \{1, {}^{i}y_0, {}^{i}y_1, \ldots, {}^{i}y_N\}.$$

TABLE 7.3. Numerical Results for Example 3.

	$10^4 \times {}^1y$				$10^4 \times {}^2y$			
x	Explicit Scheme h = 0.5	Blended DIFSUB[22] Variable h $t = 10^{-6}$	Lambert [15] h = 0.01	Theoretical Solution	Explicit h = 0.5	Blended DIFSUB [22]	Lambert [15] h = 0.01	Theoretical Solution
0.5	6.1038	6.1038	6.0731	6.0795	2.2096	2.2096	2.1467	2.1574
1.0	6.9655	6.9650	6.9427	6.9467	3.9324	3.9315	3.8854	3.8922
1.5	7.6365	7.6362	7.6175	7.6221	5.2743	5.2735	5.2371	5.2433
2.0	8.1592	8.1590	8.1444	8.1481	6.3194	6.3189	6.2901	6.2955
2.5	8.5663	8.5662	8.5555	8.5577	7.1333	7.1332	7.1106	7.1149
3.0	8.8834	8.8833	8.8741	8.8768	7.7673	7.7671	7.7492	7.7531
3.5	9.1303	9.1303	9.1263	9.1252	8.2610	8.2609	8.2592	8.2500
4.0	9.3226	9.3226	9.3238	9.3187	8.6456	8.6455	8.6525	8.6371
4.5	9.4724	9.4724	9.4765	9.4694	8.9452	8.9451	8.9564	8.9386
5.0	9.5891	9.5891	9.5945	9.5867	9.1784	9.1784	9.1915	9.1734

Example 4 (see Enright, et al. [5]

Van der Pol's oscillator (considered in Enright, et al. [6])

$$(7.4) \qquad y_1' = y_2 \qquad\qquad y_1(0) = 2$$

$$y_2' = 5(1-y_1^2)y_2 - y_1 \qquad y_2(0) = 0$$

$$0 \le x \le 1.$$

Eigenvalues: -0.067 and -15 → 5.7 and -1.5 → 3.6 and 1.4 → 2.4 ± 2.8i → -0.052 ± 8.8i → -2.0 → 9.5i → -5.9 → 4.5i → -2.0 and -12 → 0.050 and -15 → 1.1 and -3.4.

The numerical computation was effected with both the explicit and the implicit schemes using uniform mesh sizes h = 0.2, 0.15, 0.1, 0.05, 0.025 and 0.0125. The same problem was solved with the blended DIFSUB using an initial mesh size $h = 10^{-3}$ as suggested in Enright, et al. [6].

From Table 7.4 the new schemes compare favorably with the blended DIFSUB.

TABLE 7.4. Numerical Results for Example 4.

EXPLICIT

No. of Fn. Eval.	h	y(1)	y(2)
5	0.2000	1.8716065	-0.14358810
7	0.1500	1.8711045	-0.14574713
10	0.1000	1.8705973	-0.14610294
20	0.0500	1.8694380	-0.14823599
40	0.0250	1.8694389	-0.14823587
80	0.0125	1.8694388	-0.14823588

Blended DIFSUB

No. of Fn. Eval.	$h_0=10^{-3}$ $\epsilon=10^{-6}$	y(1)	y(2)
		1.86944	-0.148236

IMPLICIT

No. of Fn. Eval.	h	y(1)	y(2)
-	0.2000	*	*
-	0.1500	*	*
42	0.1000	1.8693953	-0.14824187
81	0.0500	1.8694357	-0.14823631
161	0.0250	1.8694387	-0.14823589
321	0.0125	1.8694389	-0.14823587

* No convergence

Example 5

$$(7.5a)\qquad y' = \begin{pmatrix} -10^{-5} & 100 \\ -100 & -10^{-5} \end{pmatrix} y, \qquad y(0) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \qquad 0 \le x \le 10\pi.$$

This is the model problem (1.2) with $\in = 10^{-5}$ and $\omega = 100$ whose theoretical solution is

$$(7.5b)\qquad y(x) = e^{-10^{-5}x} \begin{pmatrix} \sin 100x \\ \cos 100x \end{pmatrix}.$$

The numerical results in Table (7.5) are obtained with a uniform mesh size $h = \pi/20$ and only one evaluation of the stiffness/oscillatory parameters was obtained and given by

$$\Omega_1 = \begin{pmatrix} -10^{-5}-1000i & 0 \\ 0 & -10^{-5}-1000i \end{pmatrix}, \quad \Omega_2 = \begin{pmatrix} -10^{-5}+1000i & 0 \\ 0 & -10^{-5}+1000i \end{pmatrix}$$

TABLE 7.5. Numerical Results for Example 5.

$x_f = 10$, uniform $h = \pi/20$

x	$10^{12} \times {}^1T_{t+1}$	$10^{12} \times {}^2T_{t+1}$
π	0.16918	0.00949
2π	0.02447	0.02233
3π	0.29342	0.03504
4π	0.61126	0.04402
5π	0.92906	0.05704
6π	1.2468	0.07060
7π	1.56451	0.08478
8π	0.09729	0.09991
9π	1.29056	1.06429
10π	1.60815	0.12150

one evaluation of oscillatory/stiffness parameters

<u>Example 6</u> (Stiefel and Bettis [24])

We finally consider the nearly periodic initial value problem which was earlier studied by Stiefel-Bettis [24] and Lambert-Watson [16]:

$$(7.6a) \qquad y'' + y' = 0.001e^{ix}, \; y(1) = 1, \; y'(0) = 0.9995i, \; y \in R^1$$

whose theoretical solution is

$$(7.6b) \qquad \begin{cases} y(x) = u(x) + iv(x), & u, v \in R^1 \\ u(x) = \cos x + 0.0005x \sin x \\ v(x) = \sin x - 0.0005 \cos x \end{cases}$$

Equations (7.6b) represent motion on a perturbation of a circular orbit in the complex plane in which the point y(x) spirals slowly outwards such that its distance from the origin at any time x is given as

$$(7.6c) \qquad \tau(x) = \sqrt{(u^2(x) + v^2(x))}$$

The initial value problem (7.6a) can be expressed as

$$(7.6d) \qquad \begin{cases} {}^1y' = {}^2y & {}^1y(0) = 1 \\ {}^2y' = -{}^1y + 0.001 \cos x \;, & {}^2y(0) = 0 \\ {}^3y' = {}^4y \;, & {}^3y(0) = 0 \\ {}^4y' = -{}^3y + 0.001 \sin x \;, & {}^4y(0) = 0.9995 \end{cases}$$

The system (7.6d) was solved with the explicit formulas in the range $0 \leq x \leq 40\pi$ which corresponds to 20 orbits of the point y(x). The integration was performed using uniform mesh sized $h = \pi/4, \pi/5, \pi/6, \pi/9$, and $\pi/12$. Two sets of numerical results were generated--in the first set, the oscillatory/stiffness parameters are obtained once at the first step of integration while in the second set, the oscillatory parameters are evaluated at every step of integration.

The same problem was solved with the symmetric myltistep method of Lambert and Watson [16] as well as the Störmer-Cowell five-step multistep formula [24] (both of order 6):

(7.6e) $$y_{t+5} - 2y_{t+4} + y_{t+3} = \frac{h}{240}(18f_{t+5} + 209f_{t+4} + 4f_{t+3} + 14f_{t+2} - 6f_{t+1} + f_t).$$

The exact distance from the origin $\tau(x)$ is given by (7.6c) and the approximate distance is $\tau = \sqrt{({}^1y^2 + {}^3y^2)}$ at $x = 40\pi$. All the solutions generated by the new scheme spiral outward in agreement with the theoretical solution as well as Lambert's scheme whilst the first three values generated by Störmer-Cowell scheme spiral inward.

From the Tables (7.6a, b and c) which respectively show τ, $|\tau(x)-\tau|$ and $|\hat{y}(x)-\hat{y}| = \sqrt{[({}^1y(x)-{}^1y)^2 + ({}^3y(x)-{}^3y)^2]}$, we see that despite the fact that the new scheme is of lower order, yet it is more accurate than both the symmetric multistep method as well as the five order Störmer-Cowell multistep scheme.

TABLE 7.6a. $x_f = 40\pi$, $\tau(x_f) = 1.001972$

h	Störmer-Cowell	Symmetric	Explicit	
			one evaluation of parameters	repeated eval. of parameters
$\pi/4$	0.965645	1.003067	1.002311	1.001972
$\pi/5$	0.993734	1.002217	1.002205	1.001972
$\pi/6$	0.999596	1.002047	1.002140	1.001972
$\pi/9$	1.001829	1.001978	1.002050	1.001972
$\pi/12$	1.001953	1.001973	1.002016	1.001972

TABLE 7.6b. $x_f = 40\pi$, $\tau(x_f) = 1.001972$

h	$10^6 x \lvert\tau(x)-\tau\rvert$			$10^9 x \lvert\tau(x)-\tau\rvert$
	Störmer-Cowell	Symmetric	Explicit: one evaluation of parameters	Explicit: repeated eval. of parameters
$\pi/4$	36 327	1 095	339	204
$\pi/5$	8 238	245	233	66
$\pi/6$	2 376	75	167	26
$\pi/9$	143	6	78	3
$\pi/12$	19	1	44	0

TABLE 7.6c. $x_f = 40\pi$, $u(x_f) = 1$, $v(x_f) = 0.062832$

h	$10^6 x \lvert\hat{y}(x_f)-\hat{y}_f\rvert$			$10^9 x \lvert\hat{y}(x_f)-\hat{y}_f\rvert$
	Störmer-Cowell	Symmetric	Explicit: one evaluation of parameters	Explicit: repeated eval. of parameters
$\pi/4$	48 014	31 272	389	384
$\pi/5$	13 136	7 300	252	159
$\pi/6$	4 494	2 303	176	77
$\pi/9$	405	188	79	15
$\pi/12$	73	33	45	5

8. CONCLUDING REMARKS

The proposed explicit scheme (2.3) and (2.9) is considered to be more efficient and accurate than the DIFSUB and the blended DIFSUB for linear stiff systems of ordinary differential equations. It is equally efficient for highly oscillatory systems as it is capable of admitting fairly large mesh size and still maintains high degree of accuracy. The major drawback is the need to generate higher order derivative but automatic generation of higher order derivatives is practicable for an extensive range of problems.

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Some L-stable fourth order explicit one step numerical integration formulas which require no matrix inversion are proposed to cope effectively with systems of ordinary differential equations with large Lipschitz constants (including those having highly oscillatory solutions). The implicit integration procedure proposed in Fatunla [10] is further developed to handle a larger class of stiff systems as well as those with highly oscillatory solutions. The same pair of nonlinear equations as in [10] is solved for the stiffness/oscillatory parameters. However, the nonlinear systems are transformed into linear forms and an efficient computational procedure is developed to obtain these parameters. The new schemes compare favorably with the backward differentiation formula (DIFSUB) of Gear [12, 13] and the blended linear multistep methods of Skeel and Kong [22], and the symmetric multistep methods of Lambert and Watson [16].

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